Nuclear Lattice Simulations

Lecture 4: Applications of Nuclear Lattice Simulations

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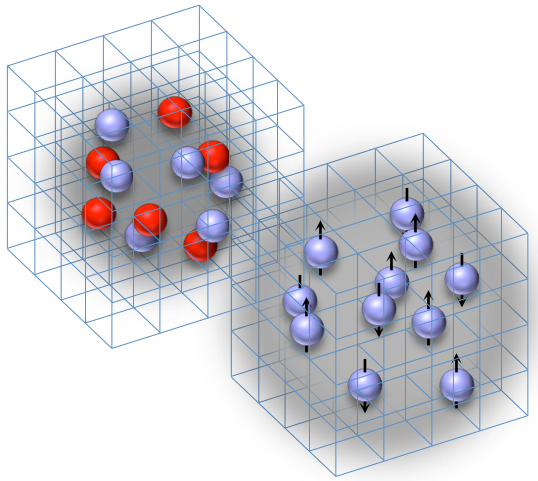


Swieca Summer School on Nuclear Theory
Campos do Jordão, SP, Brazil
Feburary 10-15, 2019

Lectures

Lecture 1: Lattice Field Theory and Monte Carlo Methods

Lecture 2: Path Integrals, Transfer Matrices, and Auxiliary Fields

Lecture 3: Chiral Effective Field Theory on the Lattice

Lecture 4: Applications of Nuclear Lattice Simulations

Adiabatic projection method

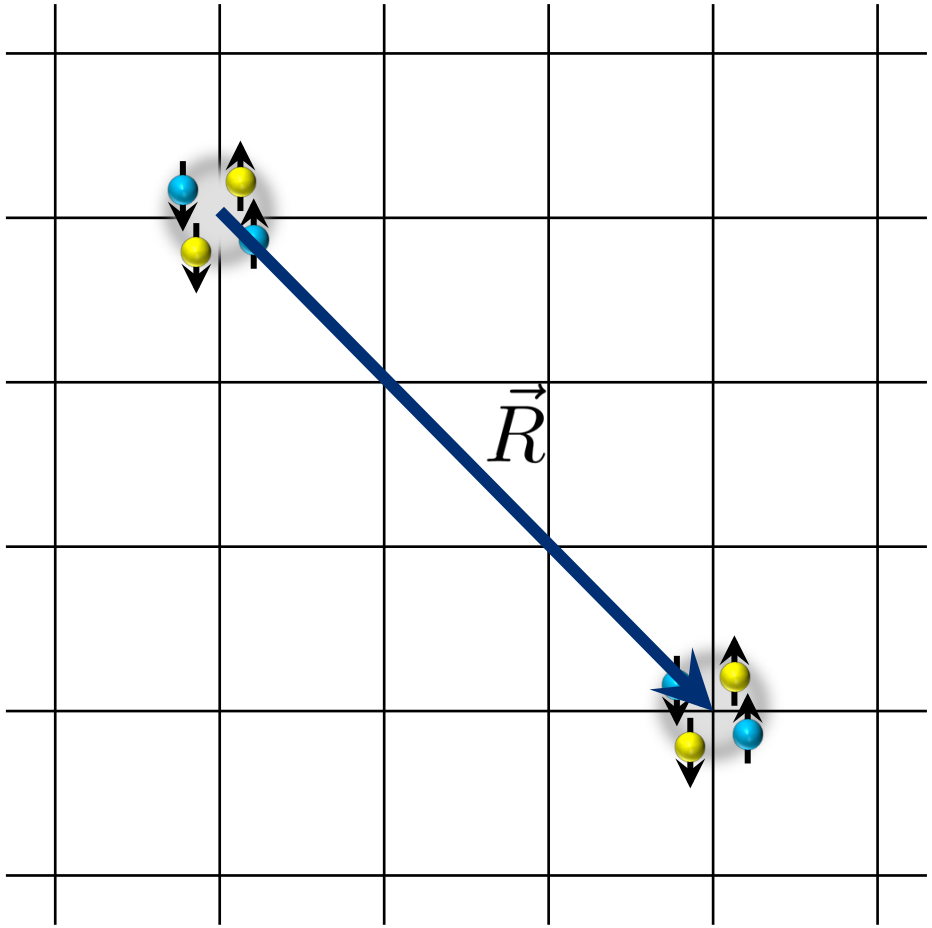
First principles method for scattering and reactions of quantum bound states using Monte Carlo simulations.

Strategy is to divide the problem into two parts. In the first part, we use Euclidean time projection and lattice Monte Carlo to derive an *ab initio* low-energy cluster Hamiltonian, called the adiabatic Hamiltonian (adiabatic transfer matrix for nonzero temporal lattice spacing).

In the second part, we use the adiabatic Hamiltonian to compute scattering phase shifts or reaction amplitudes.

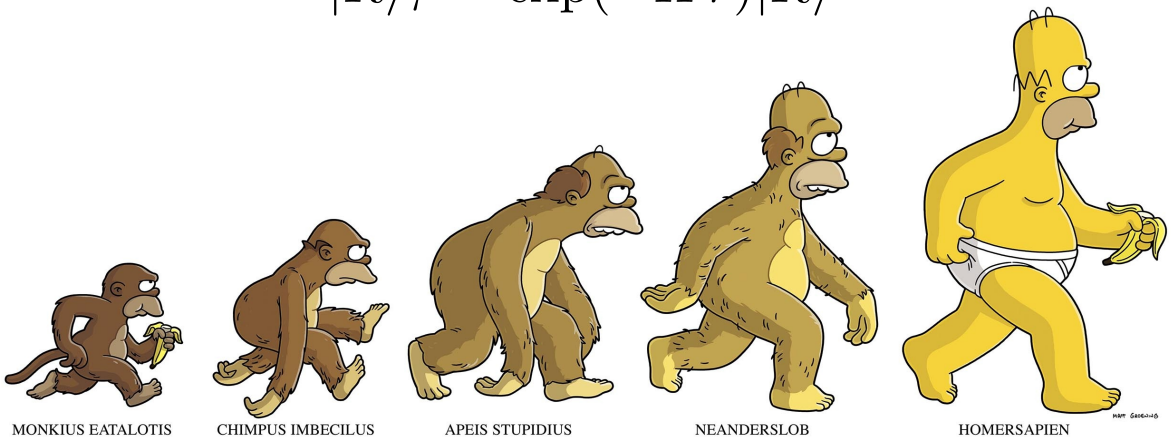
Start with localized cluster states for all possible separation vectors $\vec{R}$

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$



Cluster evolution with Euclidean time.

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$



M. Groening

For notational simplicity we use the language of continuous time evolution. The actual calculations use normal-ordered transfer matrices.

$$|\vec{R}\rangle_\tau = [: \exp(-H\alpha_t) :]^{L_t} \, |\vec{R}\rangle$$

Use projection Monte Carlo to propagate cluster wavefunctions in Euclidean time to form dressed cluster states

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

Evaluate matrix elements of the full microscopic Hamiltonian with respect to the dressed cluster states,

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau$$

Since the dressed cluster states are in general not orthogonal, we construct a norm matrix given by the inner product

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

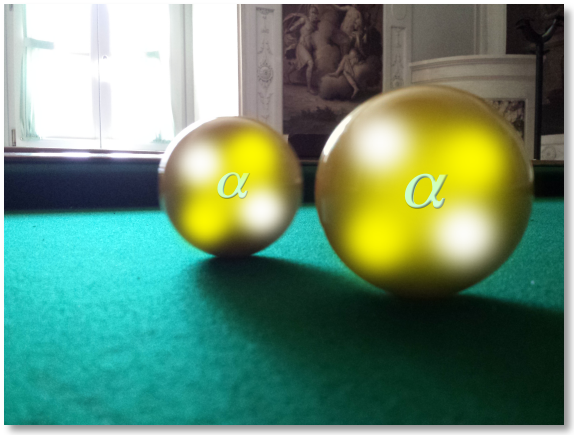
The adiabatic Hamiltonian is defined by the matrix product

$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

Distortion and polarization of the nuclear wave functions occur as we evolve in Euclidean time.

As we increase the projection time, the adiabatic Hamiltonian exactly reproduces the low-energy spectrum of the full microscopic Hamiltonian.

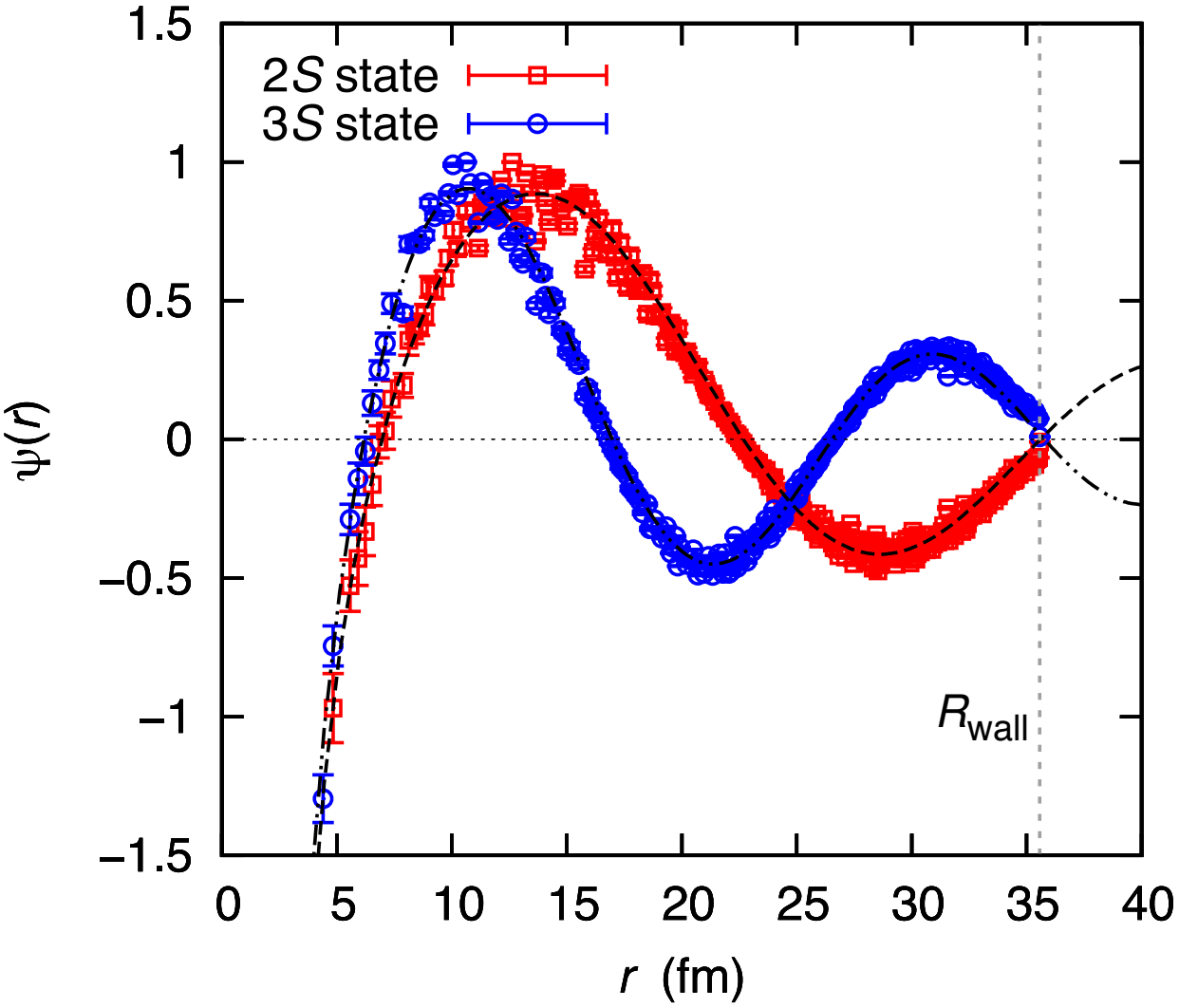
$^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$



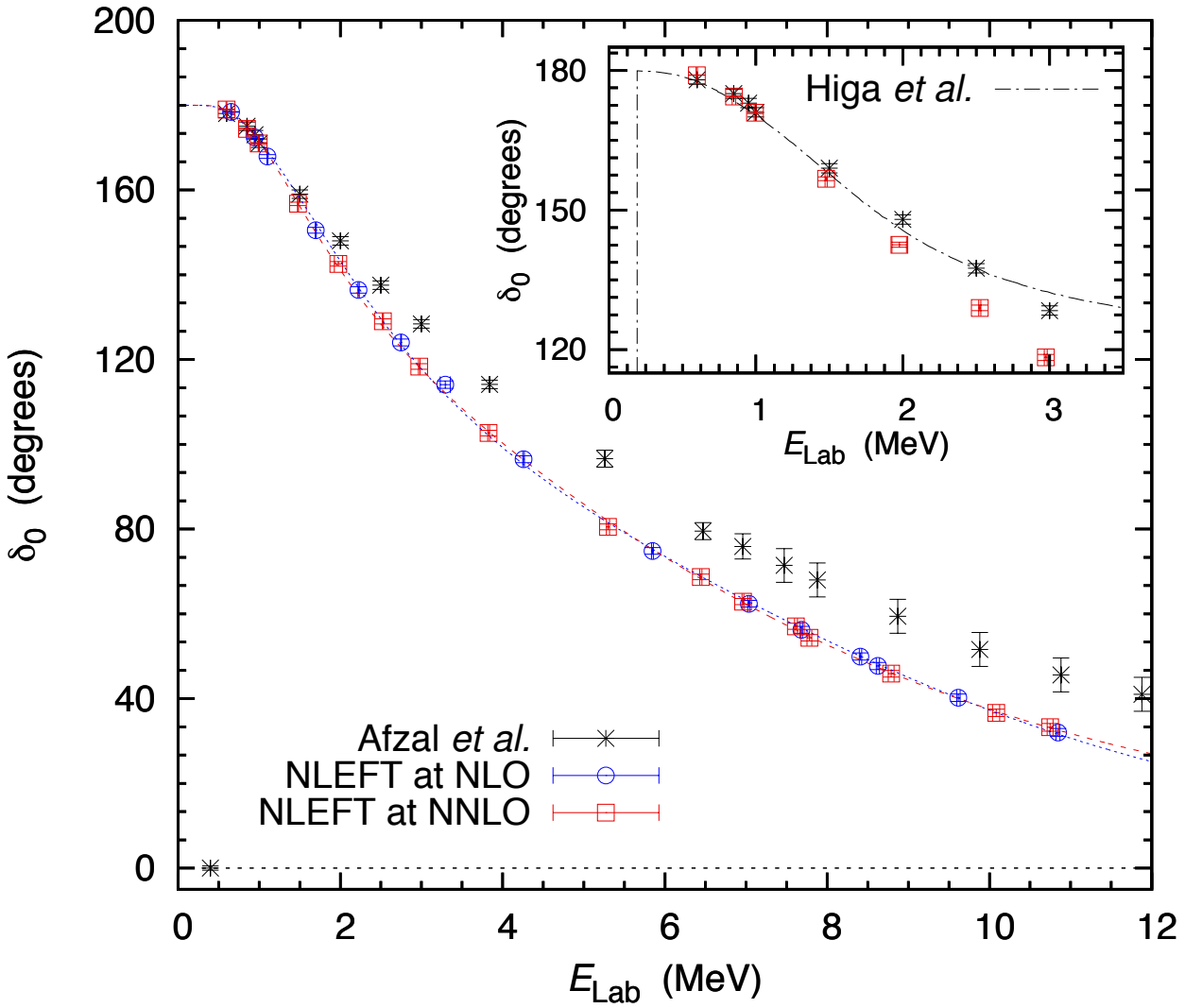
We now present *ab initio* results for alpha-alpha scattering up to NNLO with lattice spacing 1.97 fm.

Using the adiabatic projection method, we performed lattice simulations for the S-wave and D-wave channels.

Elhatisari, D.L., Rupak, Epelbaum, Krebs, Lähde, Luu, Meißner, Nature 528, 111 (2015)


2S state
3S state
1.5
1
0.5
0
−0.5
−1
−1.5
ψ(r)
0
5
10
15
20
25
30
35
40
r (fm)
R_wall

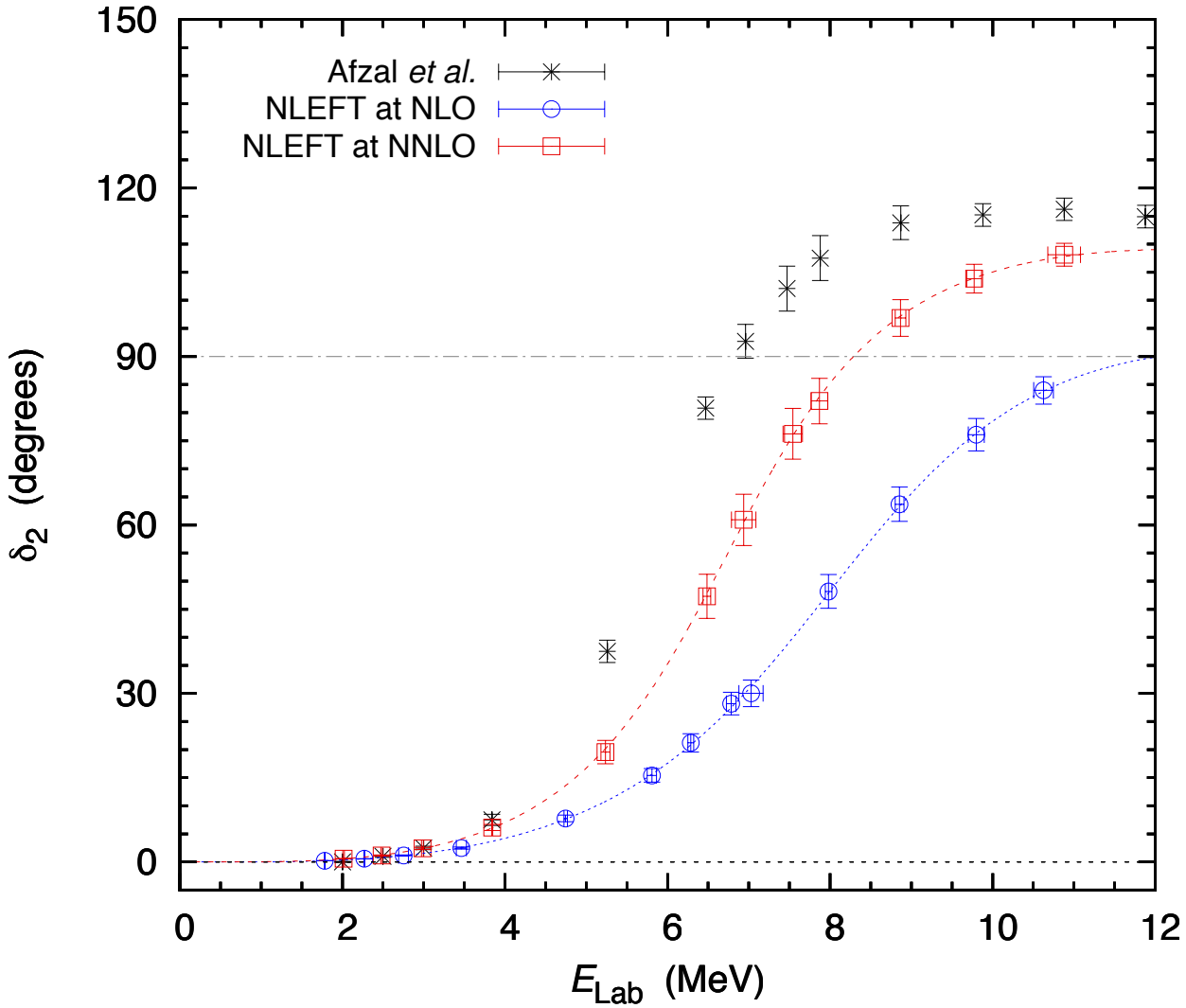
S-wave scattering



Afzal, Ahmad, Ali, RMP 41 247 (1969)

Higa, Hammer, van Kolck, NPA 809 171(2008)

D-wave scattering



Seeing Structure with Pinholes

Consider the density operator for nucleon with spin i and isospin j

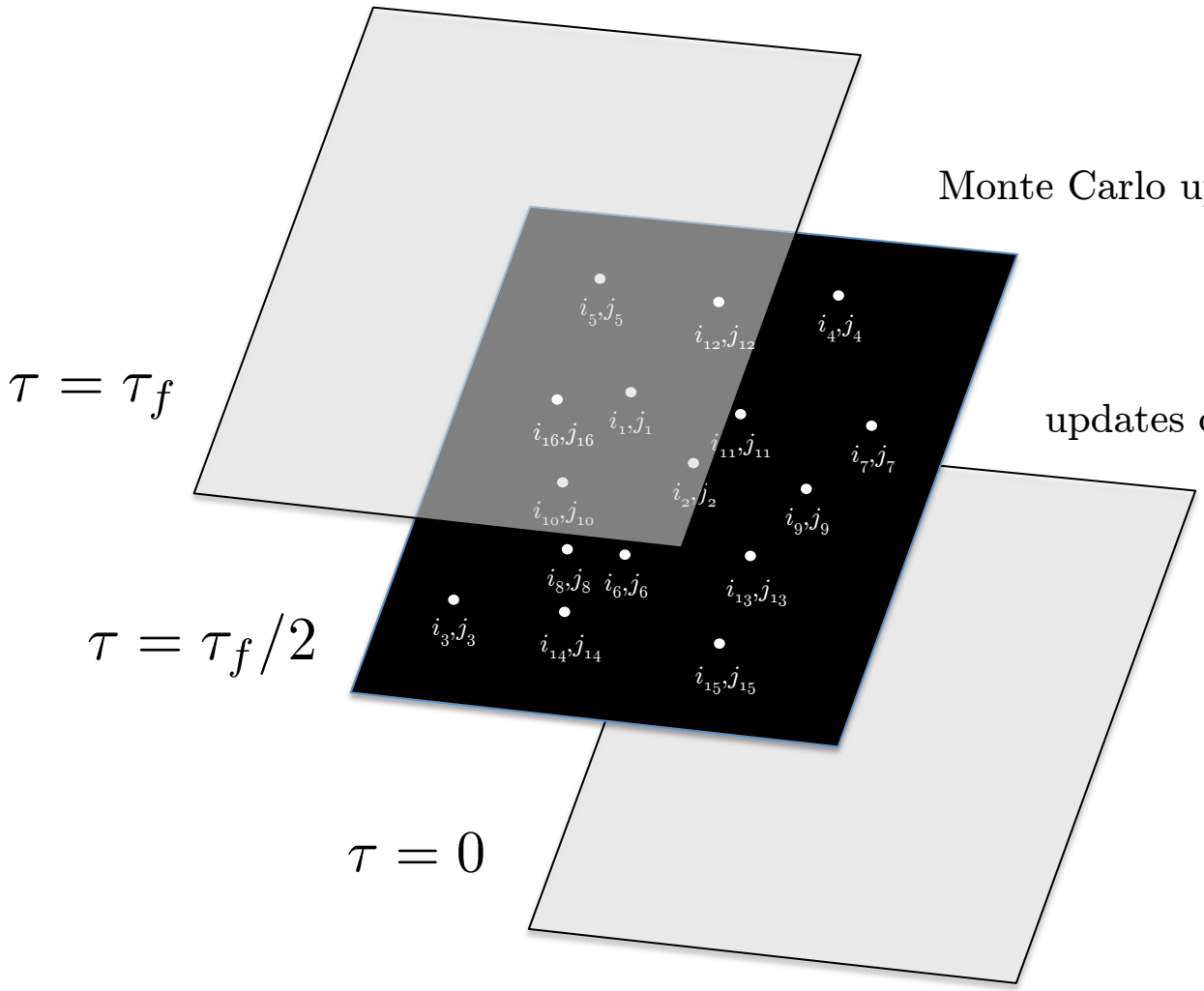
$$\rho_{i,j}(\mathbf{n}) = a^{\dagger}_{i,j}(\mathbf{n}) a_{i,j}(\mathbf{n})$$

We construct the normal-ordered A-body density operator

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$

In the simulations we do Monte Carlo sampling of the amplitude

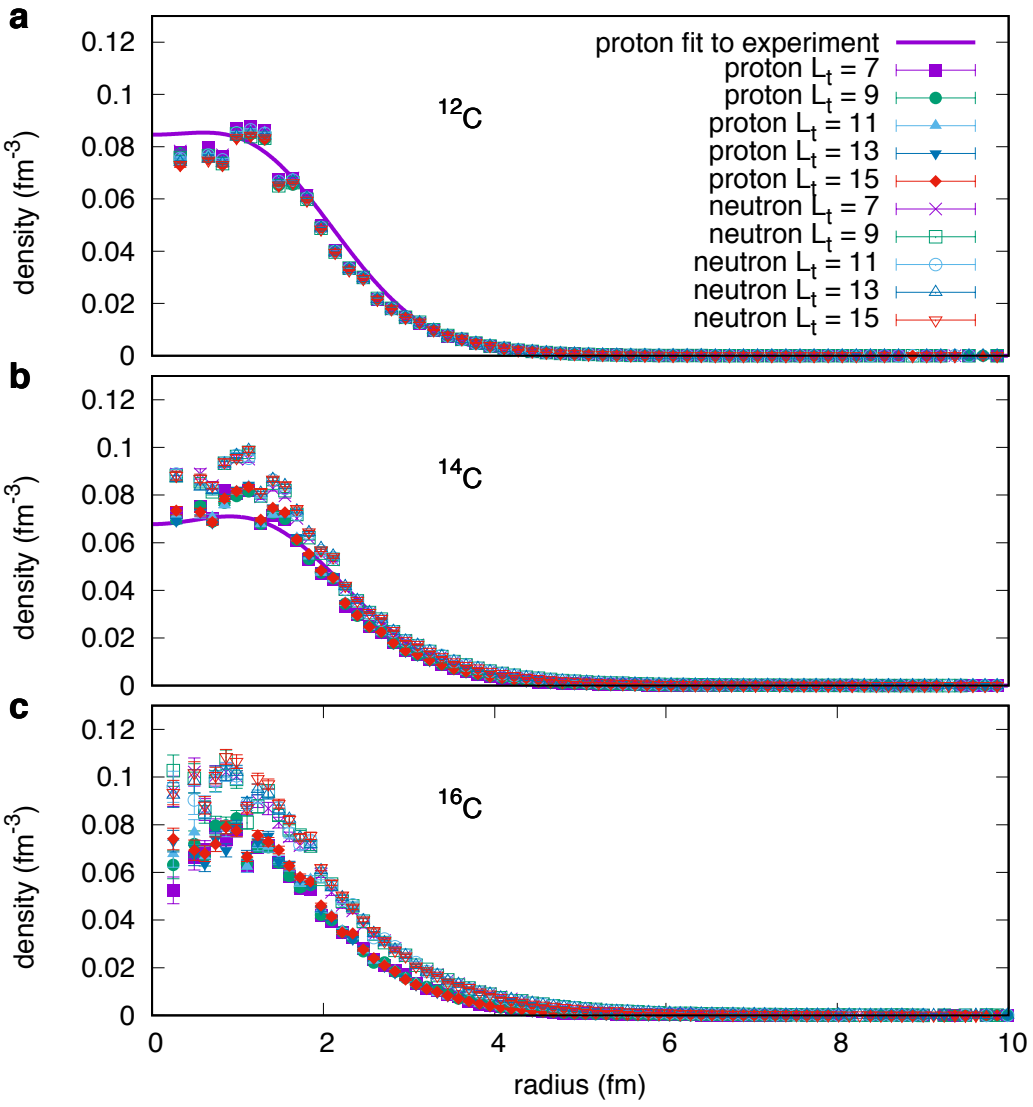
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A,t) = \langle\Psi_I|e^{-Ht/2}\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A)e^{-Ht/2}|\Psi_I\rangle$$



Monte Carlo updates of pinholes

Monte Carlo
updates of auxiliary/pion fields

Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

A Tale of Two Interactions

Two LO interactions, A and B, have nearly identical nucleon-nucleon phase shifts and well as three- and four-nucleon bound states

Nucleus	A (LO)	B (LO)	A (LO + Coulomb)	B (LO + Coulomb)	Experiment
^{8}Be	−58.61(14)	−59.73(6)	−56.51(14)	−57.29(7)	−56.591
^{12}C	−88.2(3)	−95.0(5)	−84.0(3)	−89.9(5)	−92.162
^{16}O	−117.5(6)	−135.4(7)	−110.5(6)	−126.0(7)	−127.619
^{20}Ne	−148(1)	−178(1)	−137(1)	−164(1)	−160.645

Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

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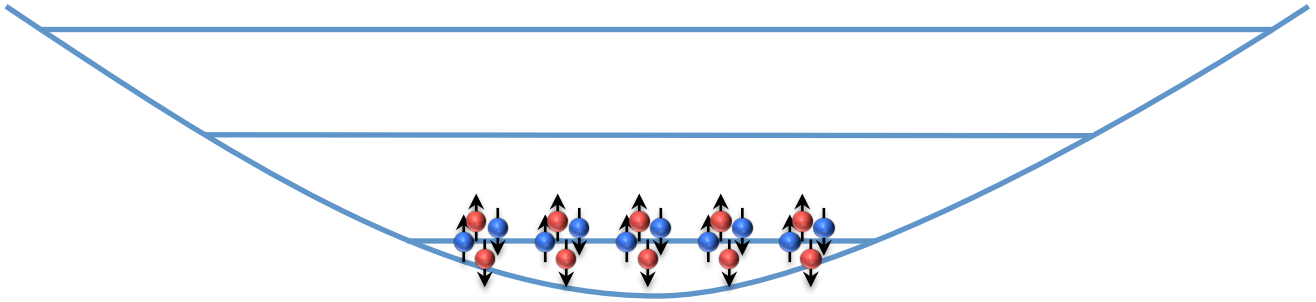
$$\frac{E_{^{8}\mathrm{Be}}}{E_{^{4}\mathrm{He}}} = 1.997(6)$$

$$\frac{E_{^{12}\mathrm{C}}}{E_{^{4}\mathrm{He}}} = 3.00(1)$$

$$\frac{E_{^{16}\mathrm{O}}}{E_{^{4}\mathrm{He}}} = 4.00(2)$$

$$\frac{E_{^{20}\mathrm{Ne}}}{E_{^{4}\mathrm{He}}} = 5.03(3)$$

Bose condensate of alpha particles!



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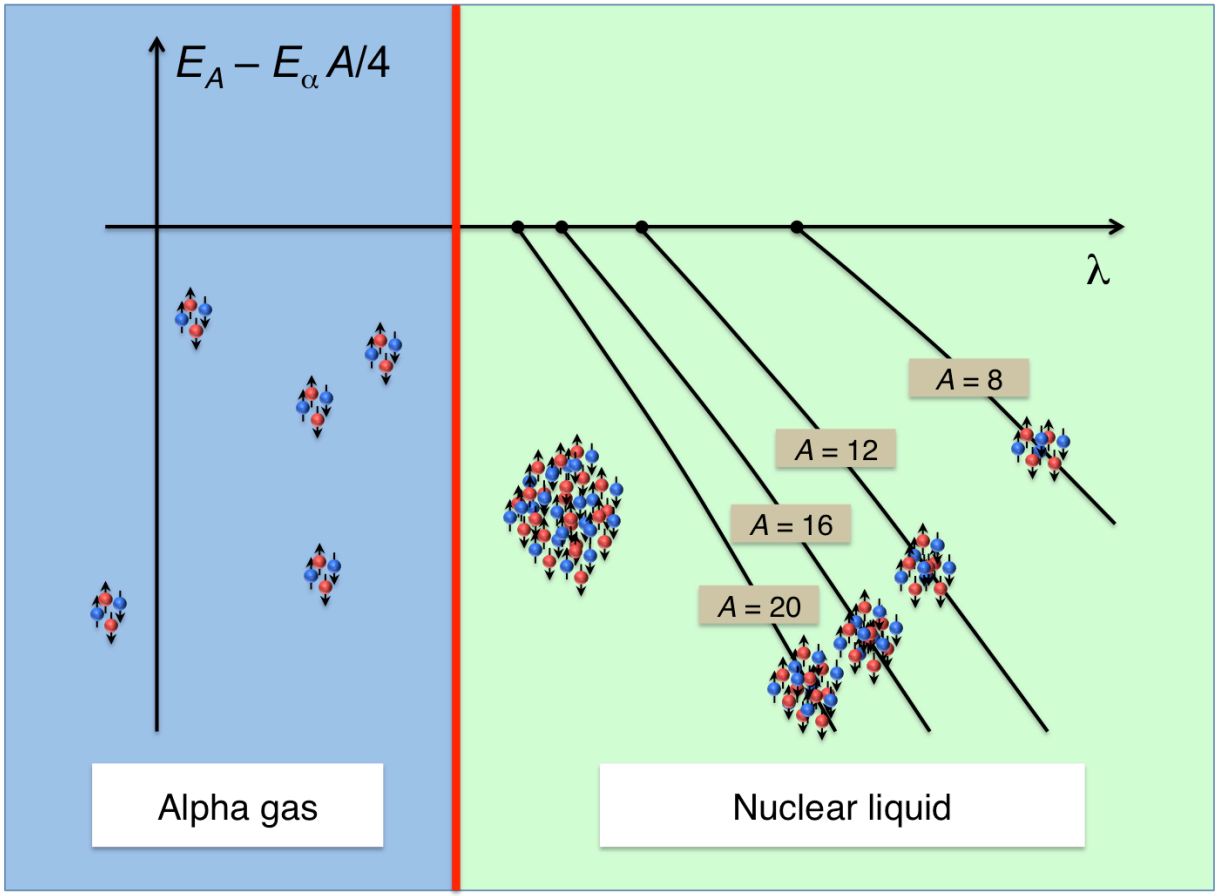
Control parameters: Sensitivity to interaction range and locality



Elhatisari, Li, Rokash, Alarcon, Du, Klein, Lu, Meißner, Epelbaum, Krebs, Lähde, D.L., Rupak, PRL 117, 132501 (2016)

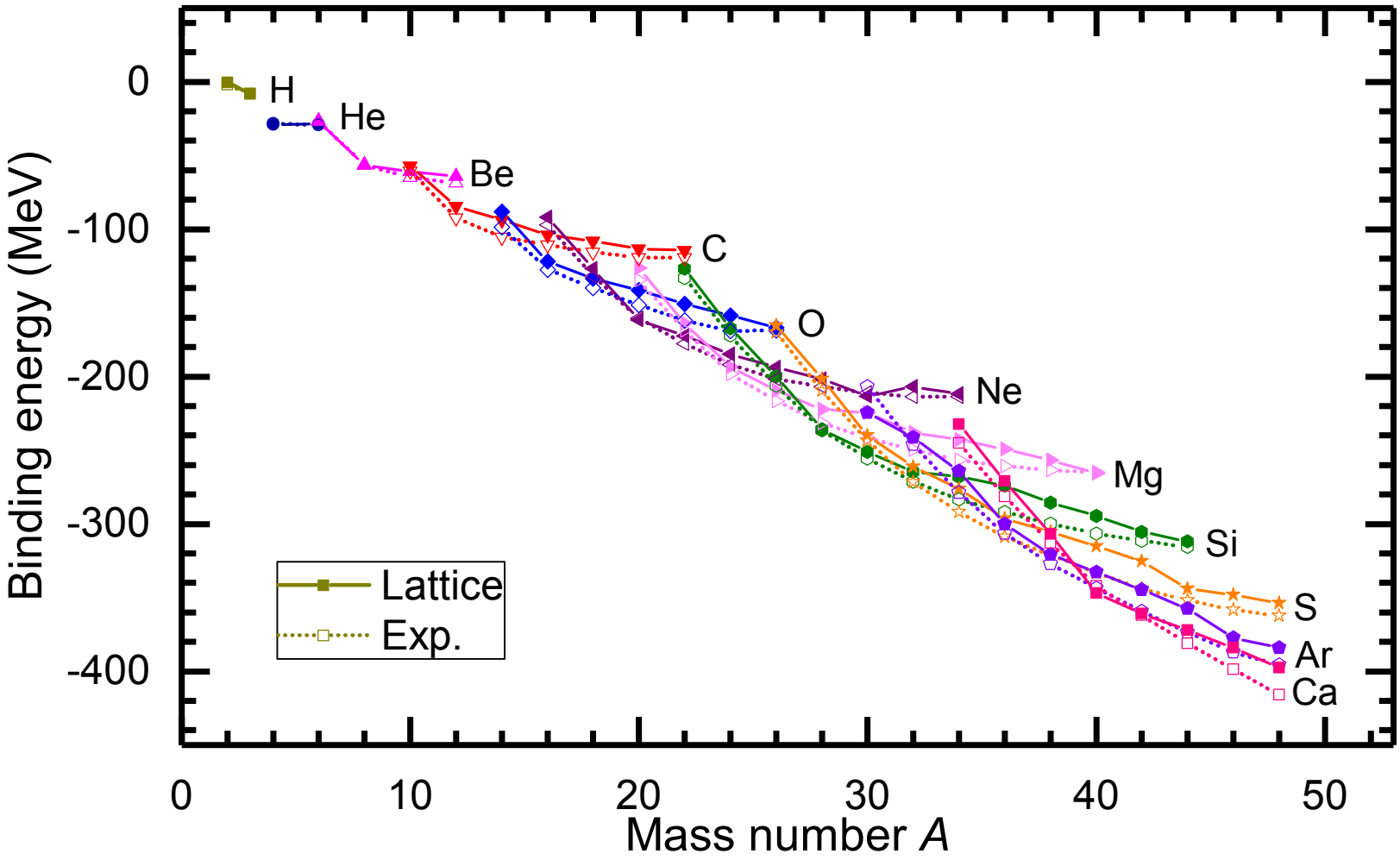
Essential Elements for Nuclear Binding

What is the minimal nuclear interaction that can reproduce the ground state properties of light nuclei, medium-mass nuclei, and neutron matter simultaneously with no more than a few percent error in the energies and charge radii?

We construct an interaction with only four parameters.

1. Strength of the two-nucleon S-wave interaction
2. Range of the two-nucleon S-wave interaction
3. Strength of three-nucleon contact interaction
4. Relative strength of the local part of the interaction

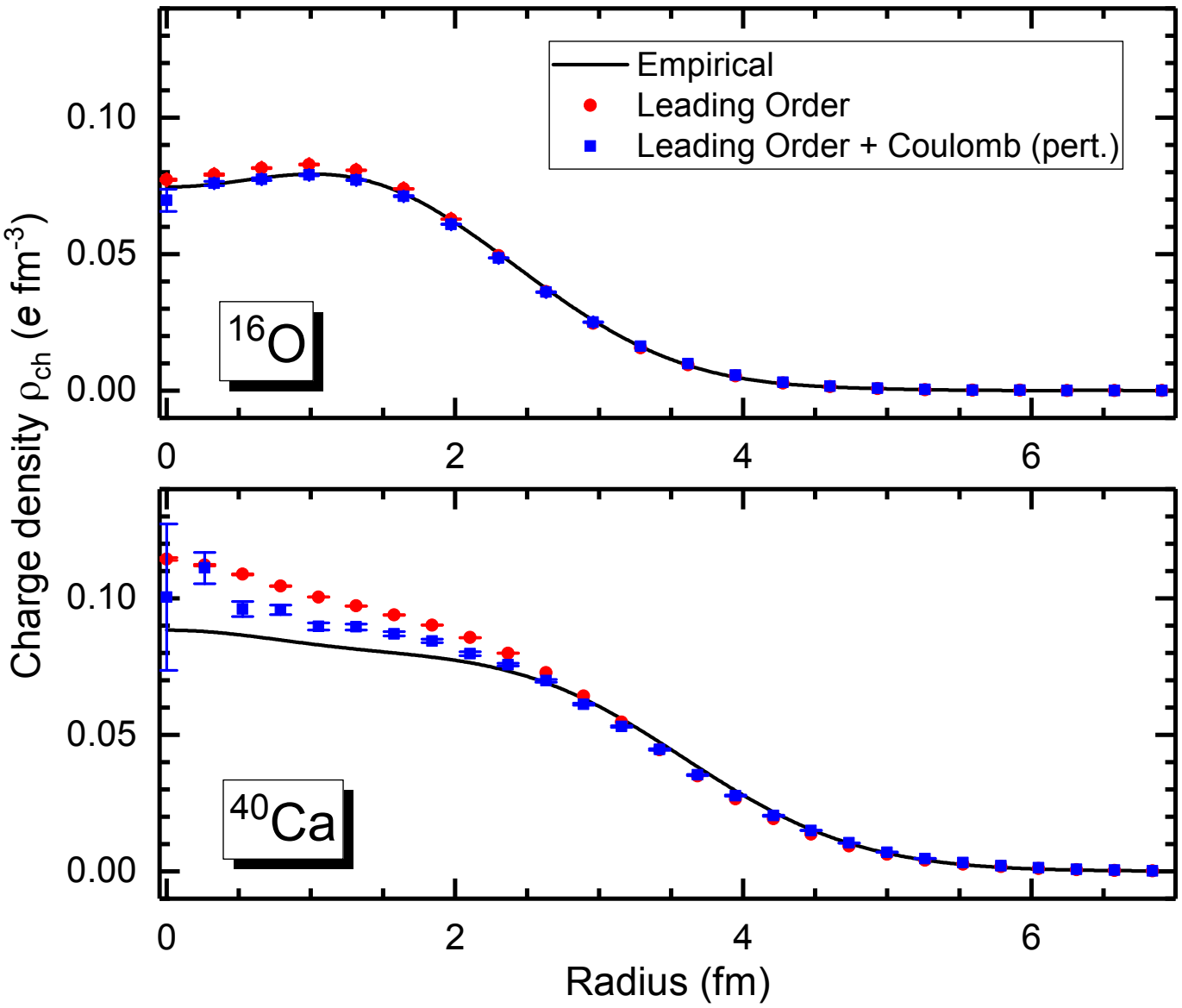
Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928



Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928

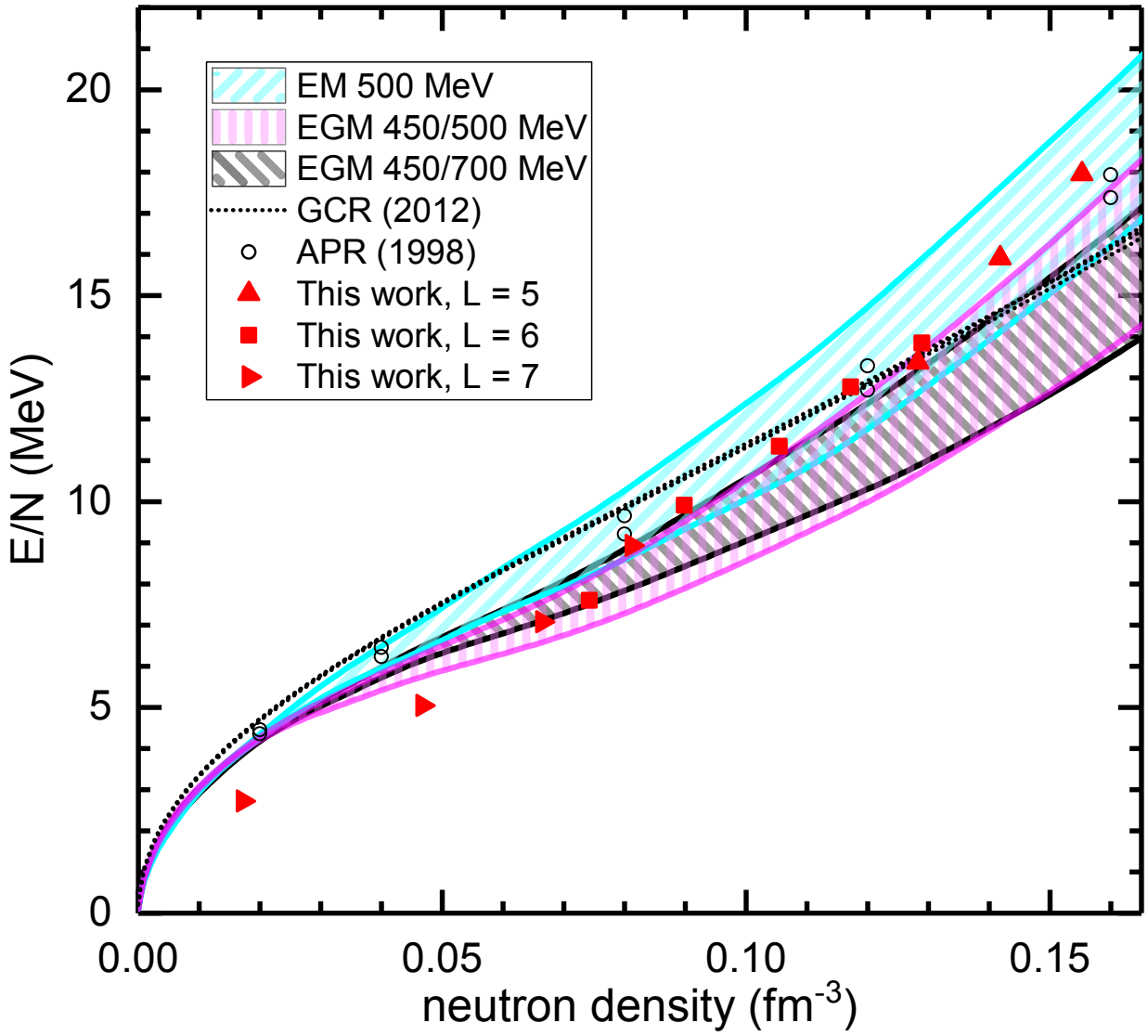
	B	Exp.	$R_{\rm ch}$	Exp.
^{3}H	8.48(2)(0)	8.48	1.90(1)(1)	1.76
^{3}He	7.75(2)(0)	7.72	1.99(1)(1)	1.97
^{4}He	28.89(1)(1)	28.3	1.72(1)(3)	1.68
^{16}O	121.9(1)(3)	127.6	2.74(1)(1)	2.70
^{20}Ne	161.6(1)(1)	160.6	2.95(1)(1)	3.01
^{24}Mg	193.5(02)(17)	198.3	3.13(1)(2)	3.06
^{28}Si	235.8(04)(17)	236.5	3.26(1)(1)	3.12
^{40}Ca	346.8(6)(5)	342.1	3.42(1)(3)	3.48

Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928



Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928

Pure neutron matter



Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, arXiv:1812.10928

Nuclear thermodynamics using pinholes

In order to compute thermodynamic properties of finite nuclei, nuclear matter, and neutron matter, we need to compute the partition function

$$\mathrm{Tr}\exp(-\beta H)$$

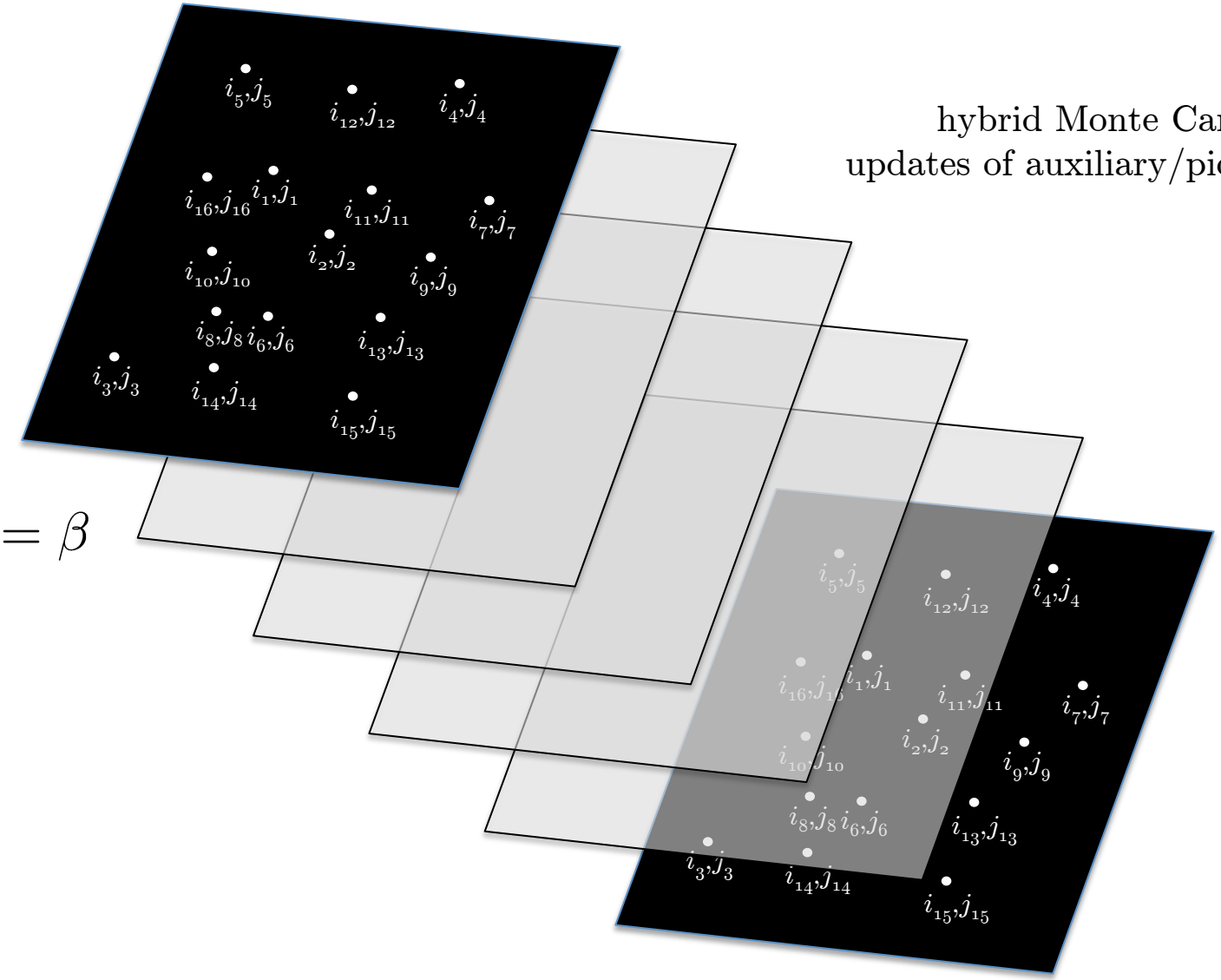
We compute the quantum mechanical trace over A-nucleon states by summing over pinholes (position eigenstates) for the initial and final states

$$\mathrm{Tr}\, O = \frac{1}{A!} \sum_{i_1 \cdots i_A, j_1 \cdots j_A, \mathbf{n}_1 \cdots \mathbf{n}_A} \langle 0 | a_{i_A,j_A}(\mathbf{n}_A) \cdots a_{i_1,j_1}(\mathbf{n}_1)\, O\, a^\dagger_{i_1,j_1}(\mathbf{n}_1) \cdots a^\dagger_{i_A,j_A}(\mathbf{n}_A) | 0 \rangle$$

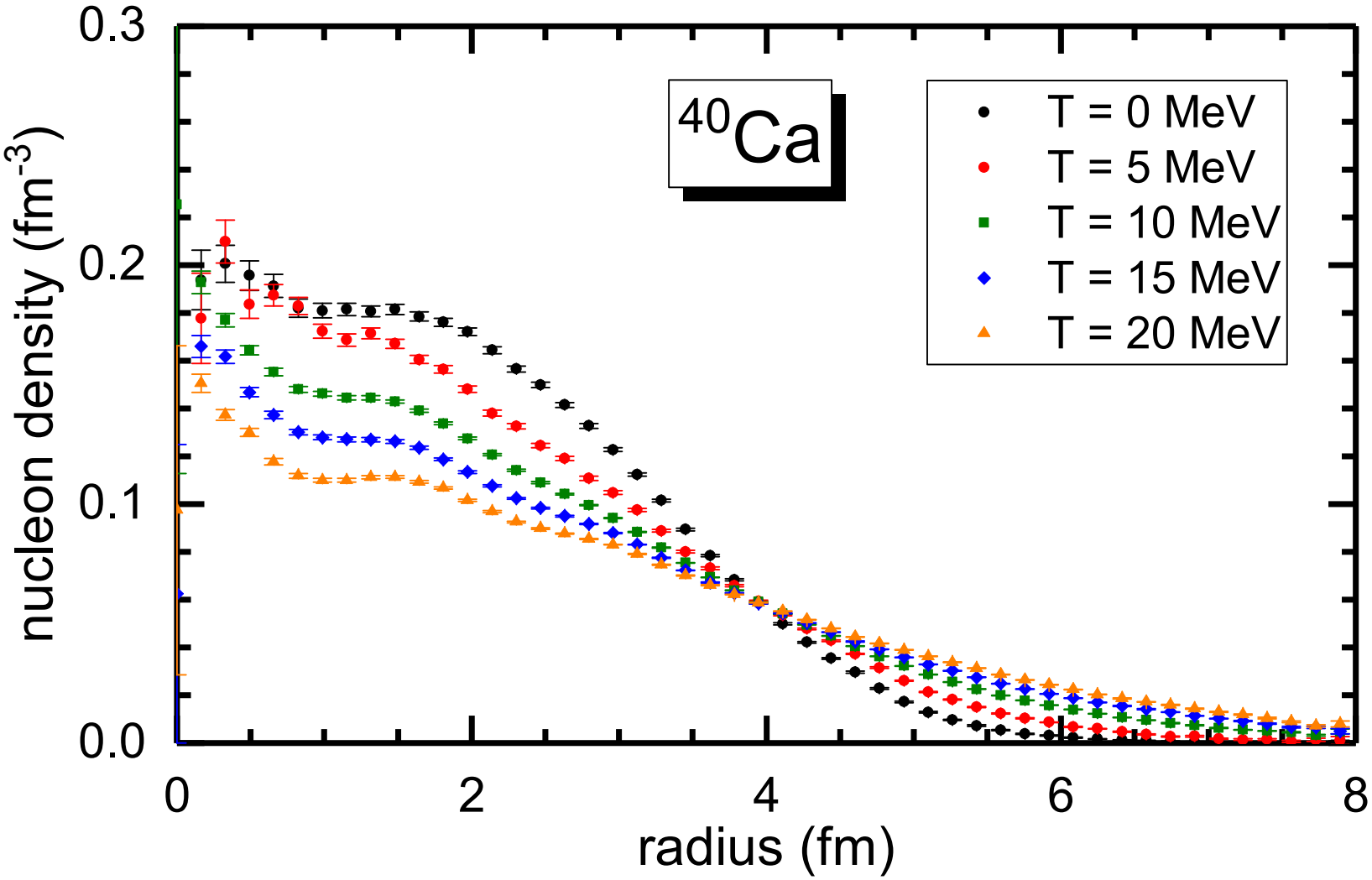
This can be used to calculate the partition function in the canonical ensemble.

Lu, *et al.*, work in progress

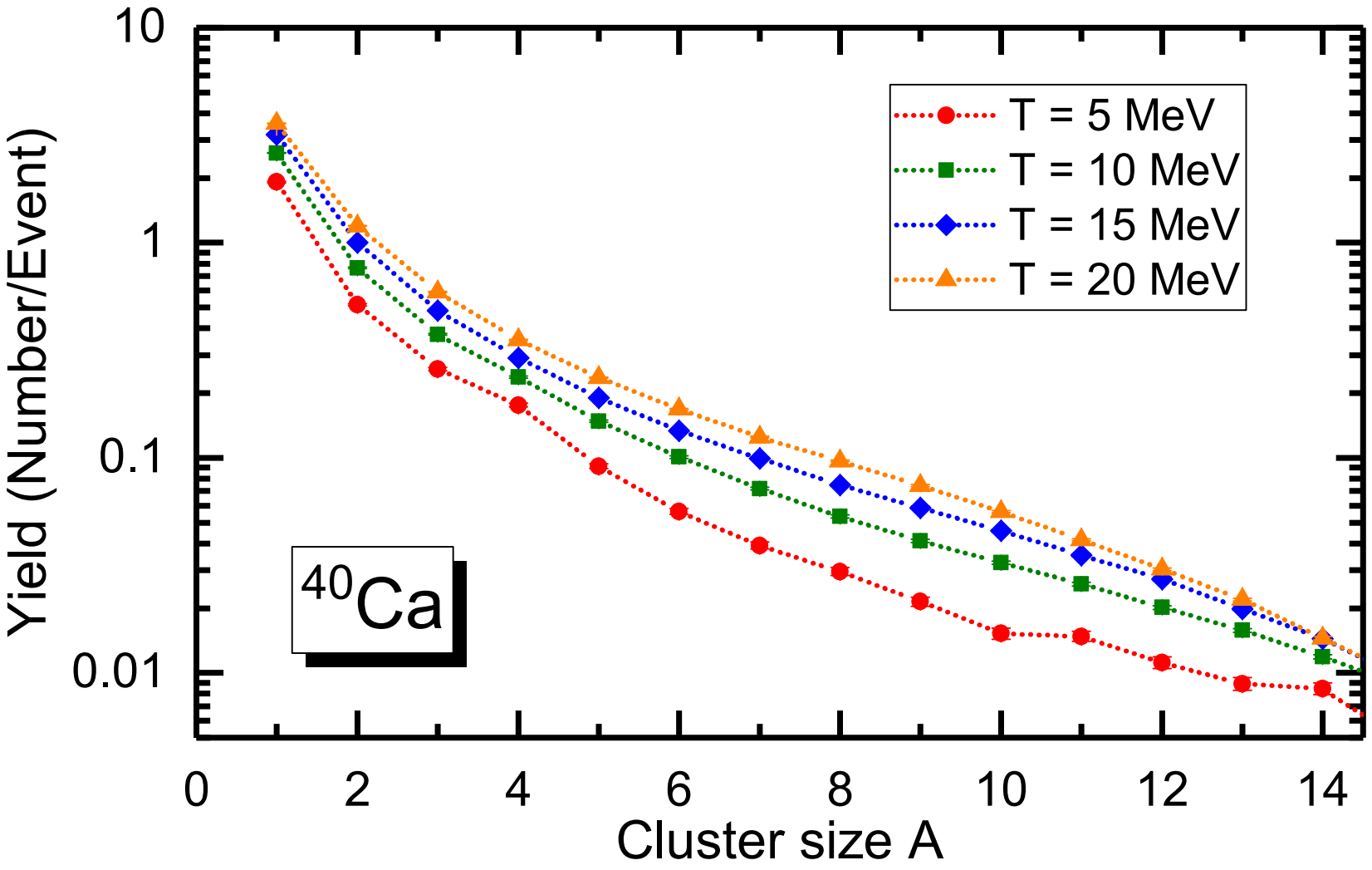
Metropolis updates of pinholes



hybrid Monte Carlo
updates of auxiliary/pion fields



Courtesy: Bing-Nan Lu



Courtesy: Bing-Nan Lu

See leedeanj.wixsite.com/leegroup for more applications.

Thanks for taking part in the Swieca Summer School!